Universal Behavior of One-Dimensional Gapped Antiferromagnets in Staggered Magnetic Field

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We study the properties of one-dimensional gapped Heisenberg antiferromagnets in the presence of an arbitrary strong staggered magnetic field. For these systems we predict a universal form for the staggered magnetization curve. This function, as well as the effect the staggered field has on the energy gaps in longitudinal and transversal excitation spectra, are determined from the universal form of the effective potential in $O(3)$-symmetric 1+1–dimensional field theory. Our theoretical findings are in excellent agreement with recent neutron scattering data on R_2BaNiO_5 ($R=$ magnetic rare earth) linear-chain mixed spin antiferromagnets.

One-dimensional isotropic Heisenberg antiferromagnets with an exchange gap in the magnetic excitation spectrum have been at the center of theoretical and experimental attention for almost two decades. This class of materials includes *integer*-spin Heisenberg chains [1] (commonly referred to as Haldane-gap systems) and half-integer spin ladders with an *even* number of legs [2]. Due to the presence of strong quantum fluctuations in these systems the staggered magnetization has a finite correlation length. The principal feature of the excitation spectrum is a degenerate triplet of sharp spin-1 excitations commonly referred to as magnons, separated from the ground state by a finite energy gap Δ. In recent years much work was aimed at understanding the behavior of such gapped 1D antiferromagnets in the presence of an external *uniform* magnetic field [3–5]. However, the effect of a *staggered* field, that couples directly to the order parameter of the classical system, has not been investigated in sufficient detail. This is mainly due to the fact that a strong magnetic field modulated on the microscopic scale was thought to be all but impossible to realize experimentally [6]. A breakthrough came with neutron scattering experiments on R_2BaNiO_5 ($R=$ magnetic rare-earth) linear-chain nickelates and their interpretation in terms of non-interacting Haldane spin chains immersed in a strong effective staggered exchange field [7,8]. In R_2BaNiO_5 compounds almost perfectly isotropic antiferromagnetic $S=1$ chains are formed by the Ni^{2+} ions. The effective staggered field is generated by the R^{3+} sublattice that becomes ordered magnetically below some Neel temperature T_N. The staggered field intensity is proportional to the magnitude of the ordered moment of R^{3+} magnetic ions and can be controlled in an experiment indirectly, by varying the temperature. One of the most significant results was the first direct measurement of the staggered magnetization curve $M_s(H_s)$ of a Haldane spin system [9]. It was found that of particular value as model systems are $(Nd_xY_{1-x})_2BaNiO_5$ species, where the effective interaction between R and Ni-sublattices is of Ising type [10], so that the transverse excitations on the Haldane chains are effectively decoupled from those on the R- subsystem. Thus the effect of the staggered field on transversal magnetic excitation spectrum of an isolated Ni^{2+} Haldane chain could be measured experimentally [10].

In [8] we gave a qualitative theoretical description of quantum disordered antiferromagnets in the presence of a staggered magnetic field and discussed the results in relevance to existing data on R_2BaNiO_5 materials. The principal conclusion was that in a weak staggered field the energy gap Δ increases in proportion to the square of induced staggered moment on the Haldane chains. It was also shown that a staggered field partially lifts the degeneracy of the magnon triplet, the gap in the longitudinal mode being three times more sensitive to H_s than that in two transversal magnons. In the present paper we refine this approach and obtain *quantitative* predictions that we directly compare to recent experimental data for $(Nd_x\ Y_{1-x})_2BaNiO_5$. We demonstrate that the behavior of both transversal and longitudinal energy gaps in the presence of a staggered field is contained in the staggered magnetization curve $M_s(H_s)$. Our central result is that for a variety of gapped one-dimensional antiferromagnets $M_s(H_s)$ has a *universal* shape defined by three experimentally accessible parameters: zero-field magnon energy gap Δ, spin-wave velocity v, and the renormalization constant Z, related to the residue of the magnon pole at $H_s=0$.

A traditional theoretical description of spin dynamics in one-dimensional quantum antiferromagnets is based on the mapping of these systems to the 1+1-dimensional $O(3)$ Non-Linear Sigma Model (NLSM) with one spatial and one temporal coordinates. This approach was first introduced by Haldane [1] for a Heisenberg antiferromagnetic spin chain, and later extended to a variety of other systems (for a recent review see [11]). Although this mapping is based on a quasiclassical approximation, and in principle it should work well only for large spins $S\gg 1$, it gives quantitatively correct predictions for any spin value. In the absence of topological term the NLSM

Lagrangian in the presence of external (staggered) field can be written as

$$\mathcal{L} = \frac{1}{2g_0} \int dx \left[\frac{1}{v_0} \left(\frac{\partial \vec{\varphi}}{\partial t} \right)^2 - v_0 \left(\frac{\partial \vec{\varphi}}{\partial x} \right)^2 + 2g_0 S \vec{H}_s \vec{\varphi} \right]. \tag{1}$$

Here $\vec{\varphi}$ is a three component unit vector ($\vec{\varphi}^2 = 1$), pointing in the direction of the local staggered moment, v_0 is the bare spin wave velocity of the system, and g_0 is the dimensionless parameter, controlling the strength of quantum fluctuations. Notice that in our notation the staggered field H_s is coupled to the local staggered *spin*. The staggered *magnetic* field $H_s^{(m)}$, coupled to local staggered magnetic moment, is proportional to H_s: $g_m \mu_B H_s^{(m)} = H_s$, where g_m is the g-factor of a magnetic ion, and μ_B is the Bohr magneton. In a large-S mapping of the Heisenberg spin chain to the NLSM [1] one has $v_0 = 2JS$, and $g_0 = 2/S$. In a more general situation these parameters should be treated as phenomenological constants fine-tuned to give the correct low energy properties of the system. The 1+1-dimensional $O(3)$ NLSM is always in a disordered state. The correlation length in the absence of staggered field is given by $\xi \sim a \exp(2\pi/g_0)$, where a is the lattice spacing. The gap Δ in the excitation spectrum is related to the correlation length via a usual relation $\Delta = \hbar v/\xi$.

In order to calculate the macroscopic properties of the system such as its staggered magnetization curve or the excitation spectrum near the AFM zone center, one needs to coarse-grain the NLSM Lagrangian by integrating out the large q and ω (small x and t) degrees of freedom. The change of parameters of the Lagrangian as a result of this coarse-graining is described by the Renormalization Group (RG) flow equations. In real space the renormalization procedure corresponds to replacing the field $\vec{\varphi}(x,t)$ with $\vec{\varphi}_r(x,t) = (v/l^2) \int_{|x'-x|<l, |t'-t|<l/v} \vec{\varphi}(x',t') dx' dt'$. It is easy to see that the coarse-grained field variable $\vec{\varphi}_r$ no longer has a well defined length. In other words, as a result of coarse-graining the NLSM Lagrangian, characterized by a rigid constraint $\vec{\varphi}^2 = 1$, becomes a "soft-spin" Lagrangian. The length of coarse-grained field variable $\vec{\varphi}_r$ has a probability distribution, defined by some effective potential. The fully renormalized Lagrangian can be written as

$$\mathcal{L} = \int dx \left[\frac{1}{2v} \left(\frac{\partial \vec{\phi}}{\partial t} \right)^2 - \frac{v}{2} \left(\frac{\partial \vec{\phi}}{\partial x} \right)^2 - U(|\vec{\phi}|) + \sqrt{Z} \vec{H}_s \vec{\phi} \right] \tag{2}$$

In this expression we have introduced the *renormalized* staggered field variable $\vec{\phi}$, defined through $\sqrt{Z}\vec{\phi} = S\vec{\varphi}$. The renormalization parameter Z was fine-tuned to give the desired form of the derivative terms, with v being the true spin wave velocity. To specify this fully renormalized Lagrangian we need to know the form of effective potential $U(|\vec{\phi}|)$. For small $\vec{\phi}$ it can be expanded in Taylor series in $\vec{\phi}^2$. The quadratic term can be written as $(\Delta^2/2v)\vec{\phi}^2$, where Δ is the true energy gap of the magnon spectrum. Indeed, the quadratic part of (2) should describe a triplet of "relativistic" non-interacting bosons. The spin wave velocity v plays the role of the speed of light in its relativistic analogue. The above form of the quadratic term correctly reproduces the spin-wave dispersion $\mathcal{E}(\pi + k) = \sqrt{\Delta^2 + v^2 k^2}$. The relativistic analogy also determines the intensity of the magnon pole in the spin correlator as

$$S^{\alpha\beta}_{SMA}(q,\omega) = \delta_{\alpha\beta} \frac{Zv}{2\mathcal{E}(q)} 2\pi \delta(\omega - \mathcal{E}(q)). \tag{3}$$

In 1+1 dimensions it is convenient to write the Taylor expansion of $U(|\vec{\phi}|)$ in terms of the set of dimensionless parameters u_{2n} defined by

$$U(|\vec{\phi}|) = \frac{\Delta^2}{v} \left(\frac{1}{2}|\vec{\phi}|^2 + \frac{1}{4!} u_4 |\vec{\phi}|^4 + \frac{1}{6!} u_6 |\vec{\phi}|^6 + \dots \right) \tag{4}$$

The effective potential, truncated at the $|\vec{\phi}|^4$ term, corresponds to the Ginzburg-Landau Lagrangian introduced by Affleck [12] on phenomenological grounds to describe Haldane-gap systems.

The *linear* staggered susceptibility at zero external staggered field can be derived from the quadratic part of Lagrangian describing non-interacting magnons. Indeed, the expectation value of $\vec{\phi}$ in the presence of a weak staggered field is easily obtained by balancing the quadratic term and the source term in Eq.(2). The result is the single mode contribution to zero-field staggered susceptibility

$$\chi^{(s)}(0) = \frac{Zv}{\Delta^2} \quad . \tag{5}$$

We can compare this prediction to the numerical results for the S=1 Heisenberg chain. Using the numerical values $Z = 1.26$ (g in their notation), $v = 2.49J$, and $\Delta = 0.41J$, reported in [13], the single mode approximation gives $\chi^{(s)}(0) \simeq 18.7/J$ in excellent agreement with Monte Carlo result $21(1)/J$ [14]. This is a manifestation of the well known fact that in Haldane-gap systems virtually all spectral weight at the AFM zone center is concentrated in the magnon triplet.

The main concern of the present paper is the *non-linear* behavior in arbitrary strong staggered fields. In order to describe these effects quantitatively one needs to know the numerical values of dimensionless couplings u_{2n}, which in principle should depend on the parameters of the bare Lagrangian. If, however, the correlation length is sufficiently long one can safely assume that these couplings are at their RG fixed point values. Fortunately, very accurate numerical values of the universal

fixed point couplings u_4, u_6, and u_8 were recently obtained by Pelissetto and Vicari in [15,16]. They carefully compared the results of ϵ, $1/N$, high temperature, and strong coupling expansions of $O(N)$-symmetric models in d dimensions with the results of Monte Carlo simulations. For $d = 2$, $N = 3$ their estimates are $u_4 = 11.8(1), u_6 = 3.33(10) \times u_4^2 = 460(20), u_8 = 20(5) \times u_4^3 = 33,000(8,000)$ [17]. In [15] the deviations of couplings from their fixed point values were estimated as $u_{2n}(\xi) - u_{2n}(\infty) \sim 1/\xi^2$. For the $S = 1$ Heisenberg antiferromagnet the correlation length $\xi \simeq 6$ (in units of lattice spacing). Therefore, one could reasonably expect the deviation of u_{2n} from their fixed point values to be around $1/36 \simeq 3\%$! This fact is confirmed numerically in Fig. 2 of [15].

From the above it follows that the quartic term $\lambda|\vec{\phi}|^4$ used by Affleck [12] to describe the effects of pairwise magnon repulsion has in fact a universal strength $\lambda = (u_4/4!)(\Delta^2/v) \simeq 0.49\Delta^2/v$. In their theoretical study of the effect of the external field on the excitation spectrum in NENP Mitra and Halperin [18] made a rough estimate of the value of λ. By matching the first term in perturbative $1/H_s$ high field expansion of the magnetization function with a small H_s expansion they have got an order of magnitude estimate, which in our notation corresponds to $\lambda \simeq Z\Delta^2/4v \sim 0.31\Delta^2/v$ rather close to our more refined result.

The effective potential manifests itself in the staggered magnetization curve of a 1D gapped antiferromagnet. Let us select z-axis along the external staggered field. The expectation value of the field $\vec{\phi}$ is defined by the minimum of the total potential energy (effective potential plus an external field term) located at $\sqrt{Z}H_s = U'(\langle\phi_z\rangle)$. Therefore, the staggered magnetization curve $M_s(H_s)$ is defined by the equation

$$H_s = \frac{1}{\sqrt{Z}} U'\left(\frac{M_s}{\sqrt{Z}}\right) = \\ = M_s \frac{\Delta^2}{Zv}\left[1 + \frac{u_4}{3!}\frac{M_s^2}{Z} + \frac{u_6}{5!}\frac{M_s^4}{Z^2} + \frac{u_8}{7!}\frac{M_s^6}{Z^3} + \dots\right]. \quad (6)$$

Using the numerical estimates for u_4, u_6, u_8 quoted above, and $Z = 1.26$ from [13], for $S = 1$ chain we obtain $\chi^{(s)}(0)H_s = M_s(1 + 1.56M_s^2 + 2.4M_s^4 + 3.27M_s^6)$ This result can be directly compared to the $M_s(H_s)$ curve measured experimentally in $\mathrm{Nd}_x\mathrm{Y}_{1-x})_2\mathrm{BaNiO}_5$ [9] (Fig. 1). The solid line is a fit to the experimental data with $\chi^{(s)}(0)$ being the only adjustable parameter. We note that the result of the fit – $\chi^{(s)}_{\mathrm{exp}}(0) = 0.53\mathrm{meV}^{-1}$ differs from the expected value $\chi^{(s)}_{\mathrm{theor}}(0) = 18.7/J \simeq 0.85\mathrm{meV}^{-1}$. It has to be emphasized however, that the experimental scaling of the abscissa in Fig. 1 in units of magnetic field heavily relies on a series of assumptions and simplifications regarding the properties of rare earth ions, and the exact applicability of the mean-field model in a wide temperature range [9]. The experimentally determined *shape* of $M_s(H_s)$, on the other hand, is a more robust result and is in excellent agreement with our theoretical predictions.

The effective potential also contains information on the behavior of the excitation spectrum in the presence of a finite staggered field. The magnon excitations are by definition deviations of local staggered magnetization from its equilibrium value. When the $O(3)$ symmetry is broken by the external field, the degeneracy of the magnon triplet is partially lifted. In this case one should distinguish between the gap $\Delta_{||}$ in the longitudinal branch of $\delta\phi_z$ excitations and the transversal gap $\Delta_\perp$ in the doublet of $\delta\phi_x$, $\delta\phi_y$ excitations. Both these gaps are determined by the quadratic terms in the expansion of $U(|\vec{\phi} + \delta\vec{\phi}|) \simeq U(|\vec{\phi}|) + \sum(\Delta_\alpha^2/2v)\ \delta\phi_\alpha^2$. After some straightforward algebra one gets $U(|\vec{\phi} + \delta\vec{\phi}|) = U\big(\sqrt{(\langle\phi_z\rangle + \delta\phi_z)^2 + \delta\phi_x^2 + \delta\phi_y^2}\big) \simeq U(\langle\phi_z\rangle) + U'(\langle\phi_z\rangle)\delta\phi_z + (U'(\langle\phi_z\rangle)/2\langle\phi_z\rangle)(\delta\phi_x^2 + \delta\phi_y^2) + (U''(\langle\phi_z\rangle)/2)\delta\phi_z^2$. The term linear in $\delta\phi_z$ is precisely compensated by $-\sqrt{Z}H_s\delta\phi_z$ coming from the external field term. The above expression for the quadratic terms in the expansion of $U(|\vec{\phi} + \delta\vec{\phi}|)$ should not come as a big surprise. Indeed, for the isotropic system the transversal staggered susceptibility in the presence of a finite staggered field H_s is given by $\chi_\perp^{(s)} = M_s(H_s)/H_s$, while the longitudinal staggered susceptibility is $\chi_{||}^{(s)} = dM_s(H_s)/dH_s$. On the other hand, in the single mode approximation one has $\chi_\alpha^{(s)}(H_s) = Zv/\Delta_\alpha^2(H_s)$. This argument again fixes the longitudinal and transversal energy gaps at

$$\Delta_\perp^2(M_s) = v\frac{\sqrt{Z}U'(M_s/\sqrt{Z})}{M_s} = \\ = \Delta^2\left[1 + \frac{u_4}{3!}\frac{M_s^2}{Z} + \frac{u_6}{5!}\frac{M_s^4}{Z^2} + \dots\right]; \quad (7)$$

$$\Delta_{||}^2(M_s) = vU''(M_s/\sqrt{Z}) = \\ = \Delta^2\left[1 + \frac{u_4}{2!}\frac{M_s^2}{Z} + \frac{u_6}{4!}\frac{M_s^4}{Z^2} + \dots\right]; \quad (8)$$

At this point it is important to see what assumptions the derivation of Eqs.(7, 8) relies on. Indeed, we implicitly assumed that the only parameter of the system which changes in the presence of staggered field are energy gaps $\Delta_\perp$, and $\Delta_{||}$. We have disregarded the changes in Z and v with field. It is well known that the spin wave velocity is not very sensitive to the parameters of the system and changes only slightly when, for instance, anisotropy is switched on [13]. This is rather natural result in field theoretical formulation of the problem since the velocity should not be renormalized at all except due to intrinsic microscopic asymmetry of spatial and temporal directions (spatial coordinate has underlying discrete lattice structure, while time is naturally continuous). The weakness of the change of Z with the field is due to the fact that in two dimensions the critical exponent η, relating

Z to the correlation length ξ as $Z \sim \xi^{-\eta}$, is equal to zero. Connecting Z to its NLSM counterpart g_0 in (1) one can approximately write $\xi \sim \exp(-2\pi/Z)$ or, alternatively, $Z^{-1}(\xi) = \text{const} - (2\pi)^{-1} \ln \xi = \text{const} + (2\pi)^{-1} \ln \Delta$. We see that a change in the gap Δ leads only to the logarithmic change in Z. Such corrections are disregarded at the precision of our calculations. In (2) the weak dependence of Z on ξ is reflected in the omission of the nonlinear terms containing derivatives of $\vec{\phi}$. It is a well know fact [19] that for small values of η this is a valid approximation. We conclude with the derivation of an explicit expression for the staggered field dependence of longitudinal and transversal gaps for $S = 1$ Heisenberg chain. Plugging the numerical values for g_4, g_6, g_8, and Z in Eqs. (7, 8) we get

$$\frac{\Delta_\perp^2(M_s)}{\Delta^2} = 1 + 1.56M_s^2 + 2.4M_s^4 + 3.27M_s^6 \tag{9}$$

$$\frac{\Delta_{||}^2(M_s)}{\Delta^2} = 1 + 4.68M_s^2 + 12M_s^4 + 22.9M_s^6 \tag{10}$$

As shown in Fig. 2, our prediction for the transversal gap is in excellent agreement with neutron scattering data on $(Nd_x\ Y_{1-x})_2BaNiO_5$ family of compounds [10], with no adjustable parameters.

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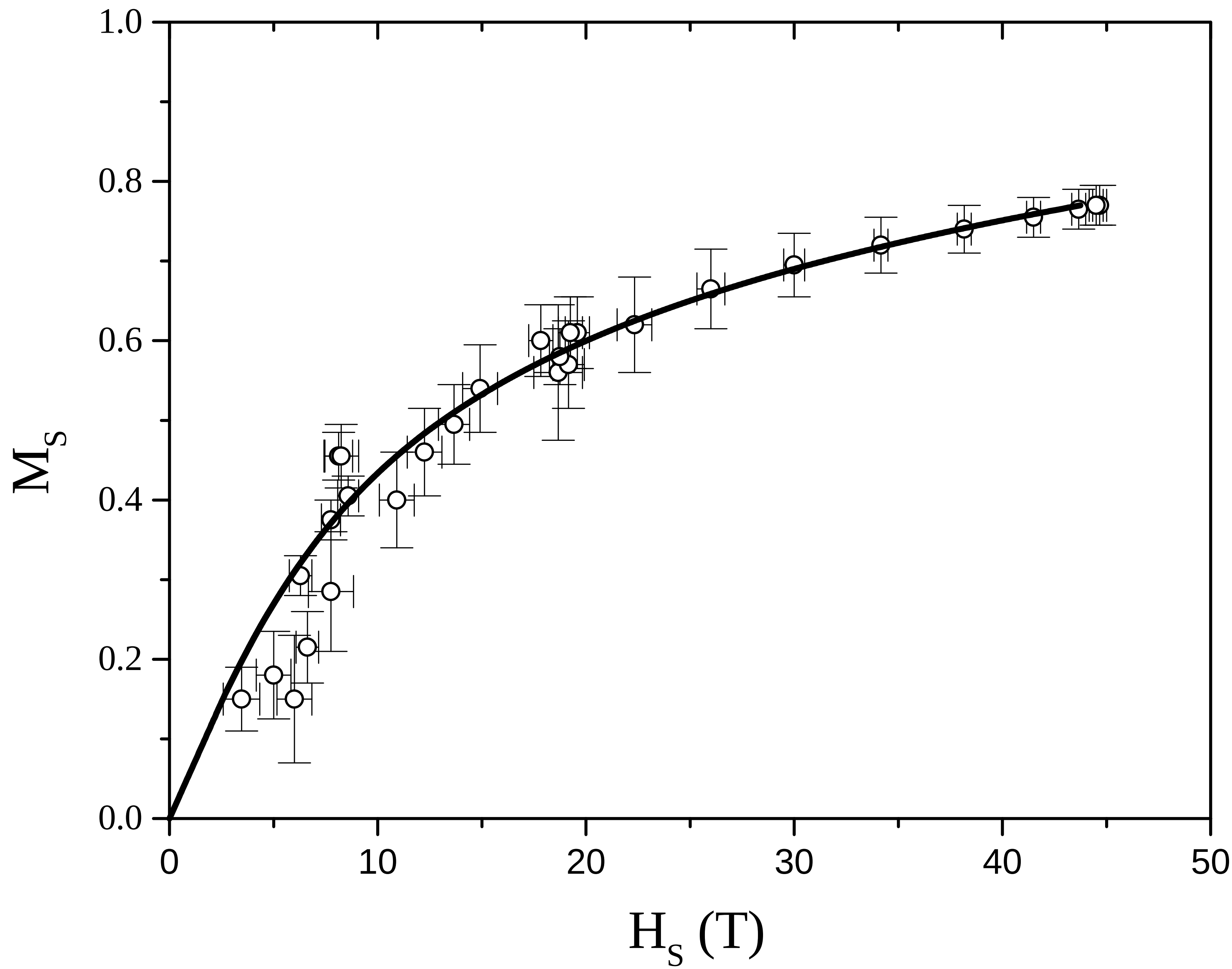
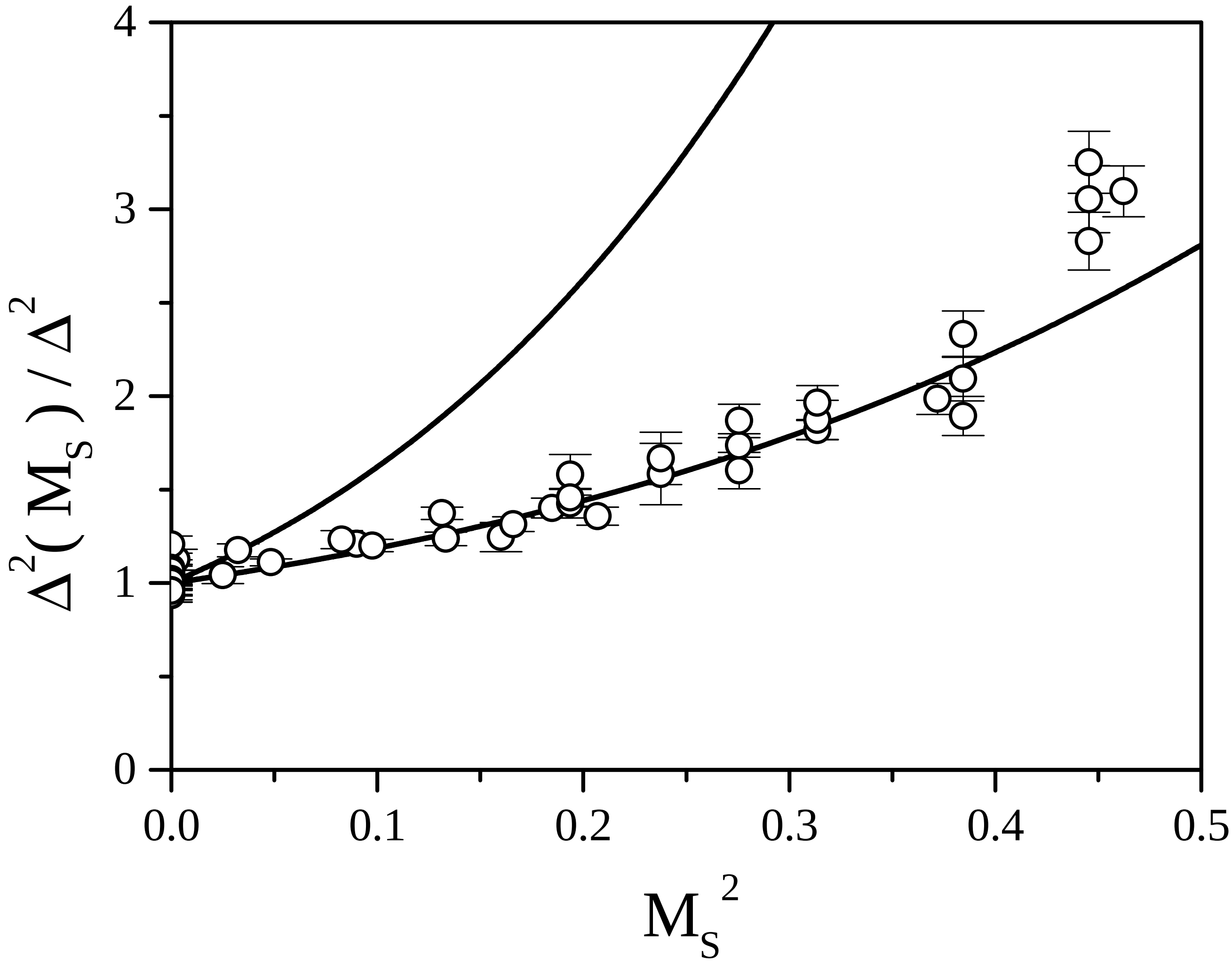
FIG. 1. The staggered magnetization curve as deduced from neutron powder diffraction data [9]) on $(Nd_xY_{1-x})_2BaNiO_5$ ($x = 0.25, 0.5, 1$). The effective staggered field is estimated through a mean-field analysis [9]. The solid line is a single-parameter fit with our theoretical result $\chi^{(s)}(0)H_s = M_s(1 + 1.56M_s^2 + 2.4M_s^4 + 3.27M_s^6)$ (see text).

FIG. 2. Inelastic neutron scattering data for the relative increase in the energy gap of the Ni-chain magnon as a function of induced staggered spin M_s in $Nd_xY_{1-x})_2BaNiO_5$ [9]. Solid lines are defined by (9,10) The experimental data agree with the theoretical prediction for the *transversal* gap.



1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
M_S
H_S (T)



4
3
2
1
0
0.0
0.1
0.2
0.3
0.4
0.5
$\Delta^2(M_S)/\Delta^2$
M_S^2